Triethylene glycol, amino, N-hexyl

Inchi: InChI=1S/C12H27NO3/c1-2-3-4-5-6-13-7-9-15-11-12-16-10-8-14/h13-14H,2-12H2,1H3
InchiKey: SZFMWHHMFMTAFY-UHFFFAOYSA-N
Formula: C12H27NO3
SMILES: CCCCCCNCCOCCOCCO
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
gf	-207.27	kJ/mol	Joback Method
hf	-654.21	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	70.24	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.182		Crippen Method
mcvol	207.530	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
tb	661.15	K	Joback Method
tc	824.78	K	Joback Method
tf	382.94	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.37	J/mol×K	661.15	Joback Method
cpg	606.81	J/mol×K	688.42	Joback Method
cpg	620.66	J/mol×K	715.69	Joback Method
cpg	633.92	J/mol×K	742.97	Joback Method
cpg	646.60	J/mol×K	770.24	Joback Method
cpg	658.70	J/mol×K	797.51	Joback Method
cpg	670.23	J/mol×K	824.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume